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DERIVATION OF THE BOHR-SOMMERFELD QUANTUM CONDITIONS FROM AN ASYMPTOTIC SOLUTION OF THE SCHROEDINGER EQUATION

by

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ABSTRACT

The Bohr-Sommerfeld quantum conditions are deduced from quantum mechanics, without recourse to separation of variables, in the limit as $\hbar$ approaches zero. Thus the conditions are obtained in the general form due to Einstein, which is applicable to non-separable classical systems, rather than in the special form due to Sommerfeld, which applies only to separable systems. Previous derivations have applied only to separable quantum mechanical systems and therefore yielded only the Sommerfeld form of the quantum conditions. The present derivation is based on an extension of the WKB method to partial differential equations, used by Dirac and others. By this method an asymptotic solution of the Schroedinger equation is constructed from which the quantum conditions follow. The asymptotic solution should prove a useful approximation in various problems. As an example, the asymptotic solution for Rutherford scattering is constructed.

I. Introduction

Bohr's quantum theory was generalized by Sommerfeld, Debye, Wilson, Epstein and Schwarzchild, and given its most general form by Einstein[1]. In each of these formulations the motion of a system was described by classical mechanics, but certain constants of the motion were restricted to be integers, or sometimes half-integers. These restrictions were called the quantum conditions. After the discovery of quantum mechanics the Bohr-Sommerfeld conditions were shown to be consequences of quantum mechanics in the limit in which Planck's constant $\hbar$ approaches zero. This demonstration was based on the WKB method and the Kramers connection formulas. Therefore it was restricted to those problems for which the Schroedinger equation was separable, and could be reduced to a system of ordinary differential equations.

The present paper presents a more general derivation of the quantum conditions from quantum mechanics, which is not based upon separation of variables. Consequently it yields these conditions in the general form given by Einstein, which is applicable to non-separable classical systems, rather than in the special form given by Sommerfeld, which applies only to separable systems. Of course the derivation yields the conditions in their corrected form, i.e., with the appropriate integer or half integer in each case. The derivation is simply related to de Broglie's condition that there must be an integral number of wavelengths along a closed orbit.

The derivation proceeds from a generalization of the WKB method to partial differential equations, given by Dirac[2]. By constructing the asymptotic solution of the Schroedinger equation according to this method, we are led to the quantum conditions.

It seems worthwhile to point out that the asymptotic solution is constructed by purely classical means, but nevertheless describes such quantum mechanical phenomena as interference. This asymptotic solution should prove as useful in many-dimensional problems as the WKB solution has proved in one dimension. As an example of the method, the asymptotic solution is constructed for the problem of Rutherford scattering, in an appendix to this article prepared with the aid of Dr. Ernest Bauer. Not only does this solution yield the correct differential scattering cross-section, as one would expect, but it also yields the logarithmic phase factor of the exact solution.

II. Asymptotic Solution of the Schroedinger Equation

Let $H(q_r,p_r,t)$, where $r = 1,\ldots, n$, be the Hamiltonian operator of a quantum mechanical system with N coordinate operators q_r and N conjugate momentum operators $p_r = -i\hbar\frac{\partial}{\partial q_r}$. In the Schroedinger representation, the state of the system is represented by a function $\psi(q_r,t)$ which satisfies the Schroedinger equation

$$(1) \qquad H(q_r,p_r,t)\psi(q_r,t) = i\hbar\,\frac{\partial\psi(q_r,t)}{\partial t}\ .$$

We wish to examine the asymptotic behavior of the solution $\psi(q_r,t,\hbar)$ of (1) as Planck's constant $\hbar$ approaches zero.

To this end we assume that as $\hbar$ approaches zero, $\psi(q_r,t,\hbar)$ has the asymptotic form $\psi_o(q_r,t,\hbar)$ given by

$$(2) \qquad \psi(q_r,t,\hbar) \sim \psi_o(q_r,t,\hbar) \equiv \sum_k A_k(q_r,t,\hbar)\exp\left[i\hbar^{-1}S_k\,(q_r,t,\hbar)\right].$$

Thus our assumption is in fact that the ratio ψ/ψ_o has the limit unity as $\hbar$ approaches zero. Furthermore we assume that the asymptotic forms of the derivatives of ψ are given by the corresponding derivatives of

ψ_o. We shall make other assumptions about ψ_o subsequently.

From the preceding assumptions it follows that ψ_o must satisfy (1) asymptotically. Thus we have

$$(3)\quad \sum_k H(q_r,p_r,t)A_k(q_r,t,\hbar)\exp\left[i\hbar^{-1}S_k(q_r,t,\hbar)\right] \sim \sum_k \exp(i\hbar^{-1}S_k)\left[i\hbar\frac{\partial A_k}{\partial t} - A_k\frac{\partial S_k}{\partial t}\right].$$

To simplify (3) we employ the identity [see Dirac, pp. 122]

$$(4)\quad H(q_r,p_r,t)\,A\exp(i\hbar^{-1}S) = \exp(i\hbar^{-1}S)H(q_r,p_r + \frac{\partial S}{\partial q_r},t)\,A.$$

Thus (3) becomes

$$(5)\quad \sum \exp(i\hbar^{-1}S_k)H(q_r,p_r + \frac{\partial S_k}{\partial q_r},t)\,A_k \sim \sum \exp(i\hbar^{-1}S_k)\left[i\hbar\frac{\partial A_k}{\partial t} - A_k\frac{\partial S_k}{\partial t}\right].$$

We now assume that (5) holds for each value of k separately. This would follow from (5) by the independence of the exponential functions if appropriate assumptions were made on the S_k, A_k and H. We thus obtain for each value of k

$$(6)\qquad H(q_r,\, p_r + \frac{\partial S_k}{\partial q_r},\, t)\,A_k \sim i\hbar\frac{\partial A_k}{\partial t} - A_k\frac{\partial S_k}{\partial t}\,.$$

Now suppose that the leading term on the left is obtained by omitting the P_r, which are proportional to $\hbar$, and that the leading term on the right is obtained by omitting $i\hbar\frac{\partial A_k}{\partial t}$. Then we assume that the remaining leading terms are not merely asymptotic, but are equal. Thus we have for each k

$$(7)\qquad H(q_r,\, \frac{\partial S_k}{\partial q_r},\, t)A_k = -A_k\frac{\partial S_k}{\partial t}\,.$$

Since the operator on the left is merely a multiplier, and since by assumption A_k is not zero, (7) becomes, for each k, an equation for S_k:

$$(8)\qquad H(q_r,\, \frac{\partial S_k}{\partial q_r},\, t) = -\frac{\partial S_k}{\partial t}\,.$$

Equation (8) is just the Hamilton-Jacobi equation for a classical mechanical system with Hamiltonian H. However we may consider complex solutions of (8) in addition to the real ones employed in classical mechanics.

We now assume that the next lower order terms in (6) are also equal. This implies that the other terms of ψ, not contained in ψ_0, do not contribute to this order in the Schroedinger equation. Then expanding H to first order in the p_r we obtain, for each k, an equation for A_k:

$$(9) \qquad -i \sum_{r=1}^{N} \left[\frac{\partial A_k}{\partial q_r} \frac{\partial H(q_r, \frac{\partial S_k}{\partial q_r}, t)}{\partial p_r} + \frac{1}{2} A_k \frac{\partial^2 H(q_r, \frac{\partial S_k}{\partial q_r}, t)}{\partial q_r \, \partial p_r} \right] = i \frac{\partial A_k}{\partial t} .$$

Multiplying by $-2iA_k$ we have instead of (9)

$$(10) \qquad \frac{\partial A_k^2}{\partial t} + \sum_{r=1}^{N} \frac{\partial}{\partial q_r} \left[A_k^2 \frac{\partial H(q_r, \frac{\partial S_k}{\partial q_r}, t)}{\partial p_r} \right] = 0.$$

If we define $P_k(q_r, t)$ by $P_k = A_k^2$ and $v_r = \frac{\partial H}{\partial p_r}$, then (10) becomes an equation for $P_k(q_r, t)$:

$$(11) \qquad \frac{\partial P_k}{\partial t} + \sum_{r=1}^{N} \frac{\partial}{\partial q_r} \left[v_r P_k \right] = 0.$$

Equation (11) is a special form of the Liouville equation of classical statistical mechanics for the probability distribution P_k of a classical mechanical system with Hamiltonian H. The specialization results from the fact that P_k depends only upon q_r and t, but not on v_r or p_r as is usual in classical mechanics. This is a consequence of the fact that quantum mechanics does not yield joint probability distributions of conjugate variables. It is also to be noted that P_k is not necessarily positive, nor even real in the present case.

The preceding derivation of (8), (11) is essentially that of Dirac, [pp. 121-3].

III. The "Classical ψ Function"

The asymptotic solution ψ_0, which ψ approaches as $\hbar$ tends to zero, can be constructed by classical mechanical considerations, since the S_k satisfy the Hamilton-Jacobi equation and the A_k^2 satisfy the Liouville equation. Nevertheless the probabilities computed from $|\psi_0|^2$ still show quantum mechanical interference effects if the sum in (2) contains more than one term.

If only one term occurs in (2), then $|\psi_0|^2=|A_1|^2 \exp(-2\hbar^{-1})\mathrm{Im}S_1$, and the probability, as well as ψ_0 itself, is exponentially damped in regions where $\mathrm{Im}S_1 > 0$. The probability in such regions vanishes as $\hbar$ tends to zero; this corresponds to the fact that these regions are excluded in classical machanics, as can also be seen from the fact that the solution of the Hamilton-Jacobi equation is not real in these regions. The exponential tail shows that ψ_0 describes such quantum mechanical effects as "tunneling".

If $\mathrm{Im}S_1 = 0$ and $|A_1|^2=A_1^2= P_1$, then $|\psi_0|^2 = P_1$. Thus as $\hbar$ tends to zero the quantum mechanical probability distribution approaches that given by the Liouville equation of classical statistical mechanics, and we may say that quantum mechanics approaches classical statistical mechanics as $\hbar$ tends to zero. The customary statement that quantum mechanics approaches classical mechanics is thus not strictly correct, but holds only when the initial data are such that $P_1 = 0$ except on one trajectory, in which case classical statistical mechanics reduces to classical mechanics. Since the classical method of computing differential scattering cross-sections is actually based on classical statistical mechanics, the preceding considerations show that the quantum mechanical cross-sections will approach those obtained by the classical method as $\hbar$ tends to zero.

The asymptotic solution ψ_0, which may be called the "classical ψ function", can be constructed by solving ordinary differential equations alone. To construct ψ_0 one may first determine the characteristics of the Hamilton-Jacobi equation, which are just the trajectories of the classical system in phase space. Then each S_k can be obtained by integration, and the A_k can also be found by solving an ordinary differential equation related to the trajectories.

As an example let us consider the case in which H is independent of t and therefore H = E, where E is a constant, the total energy of the system. Now if $q_r(t)$, $p_r(t)$ denote a trajectory, then the function S_k is given at any point of the trajectory in terms of its value $S_k(0)$ at some fixed point on the trajectory:

$$(12) \qquad S_k(q_r,t,\hbar) = S_k(0) + \int_0^t \sum_{r=1}^{N} p_r(\tau) \frac{dq_r(\tau)}{d\tau} \, d\tau - Et$$

$$= S_k(0) + \int_0^t \sum_{r=1}^{N} p_r dq_r - Et.$$

Equation (11) for P_k can also be solved at once if P_k is independent of t, for then it becomes

$$(13) \qquad \sum_{r=1}^{N} \frac{\partial}{\partial q_r} \left[v_r P_k \right] = 0.$$

Equation (13) asserts that the probability flux is divergenceless, and therefore by applying Gauss' theorem to a tube of trajectories we obtain

$$(14) \qquad P_k v \frac{d\sigma}{d\sigma_0} = P_k(0) v_0 .$$

In (14), $v = \left[\sum_{r=1}^{N} v_r^2 \right]^{1/2}$, and $d\sigma$ is the normal cross-sectional area of the tube of trajectories, both evaluated at the same point at which P_k is evaluated. The corresponding quantities v_0, $d\sigma_0$ and $P_k(0)$ are evaluated at some other point on the same trajectory, and thus (14) merely asserts the conservation of "probability". Actually (14) holds in the limit as $d\sigma_0$ tends to zero, in which case $\frac{d\sigma}{d\sigma_0}$ denotes the Jacobian of the mapping of one cross-section onto another by means of trajectories.

The problem of Rutherford scattering is treated in the appendix by means of equations (12) and (14).

IV. The Quantum Conditions

Quantum mechanics requires that ψ be a single-valued function of the q_r, and thus ψ_0 must satisfy the same condition. Therefore if the terms in ψ_0 are independent, each of them must be single-valued. Now suppose, first, that A_k is single-valued. Then $\exp(i\hbar^{-1}S_k)$ must be single-valued, which is obviously the case if S_k is single-valued. However, even if S_k is not single-valued the exponential function of S_k will still be so provided that

$$(15) \qquad \hbar^{-1} \Delta S_k = n \,.\, 2\pi, \text{ or } \Delta S_k = n\hbar . 2\pi = nh$$

In (15) $\Delta S_k(q_r, t, \hbar)$ denotes the difference between any two values of S_k at q_r, t, and n is an integer. Equation (15) may be called the "quantum condition".

If ψ denotes a steady state of energy E, then S_k is given by (12) and $A_k^2 = P_k$ is given by (14). The difference $\Delta S_k(q_r,t,\hbar)$ is then given by a line integral over some closed curve starting and ending at q_r, and (15) becomes

$$\oint \sum_r p_r dq_r = n\hbar . \tag{16}$$

In fact (16) must hold for every closed curve in the q_r space since only then will $\exp(i\hbar^{-1}S_k)$ and thus ψ_0 be single-valued at every point.

Equation (16) is exactly the quantum condition postulated by Einstein. Einstein also pointed out that since $p_r = \partial S_k/\partial q_r$, the line integral in (16) has the same value for all curves which can be deformed into each other without crossing a singularity of the integrand. For example, the integral is zero for a curve which can be deformed into a point. There are usually a *finite number* of classes of independent curves which cannot be deformed into a point. Any other curve is deformable into a linear combination of such curves with integer coefficients. Thus (16) will be satisfied for all curves if it is satisfied by one curve in each of the independent classes of irreducible curves. Thus we have, in general, a finite number of "quantum conditions", in which the integers n may be different from each other.

Einstein also pointed out that $\sum_r p_r dq_r$ is invariant under a contact transformation of variables, and therefore so are the conditions (16). He also indicated how condition (16) reduces to the Sommerfeld-Wilson quantum conditions if the system has N integrals which permit each p_i to be expressed in terms of the corresponding q_i alone (i.e., if the variables separate in the Hamilton-Jacobi equation).

It should be pointed out that the integrals (16) in the q_r space are most easily understood if that space is made into a Riemann space (i.e., multisheeted space) on which the p_r are single-valued functions of the q_r.

Let us now consider the case in which A_k is not single-valued. If ψ denotes a steady state then A_k is given by $(P_k)^{1/2}$, where P_k is given by (14). If A_k is multiple-valued at a point then one trajectory must pass through the point more than once. If different trajectories pass through the point, they are associated with different terms in ψ_o. Suppose a trajectory passes through a point q_r twice, and closes (i.e., has the same direction both times at q_r). Then v and $d\sigma$ return to their original values at q_r. But P_k may not return to its original value if either v or $d\sigma$ has vanished on the trajectory.

Such points at which v or $d\sigma$ vanishes are called caustic points in optics. At them P_k becomes infinite according to (14). This indicates that a different asymptotic expansion of the solution is required in these places. But nevertheless since v or $d\sigma$ changes sign on passing through zero, so does P_k usually. Thus if v and $d\sigma$ return to their original values after traversing a closed trajectory, P_k must undergo an even number of sign changes, and therefore A_k must change its argument by an even multiple of $\pi/2$, or by an integral multiple of π. Thus the two values of A_k will differ by $e^{i\pi}$. Then $A_k \exp(i\hbar^{-1}S_k)$ will be single-valued if

$$(17) \qquad \hbar^{-1} \Delta S_k = n2\pi + \pi \text{ , or } \Delta S_k = (n + 1/2)h.$$

Thus in this case we obtain the half-odd integer quantum condition, for curves deformable into the trajectory considered.

It is clear that the appropriate quantum condition in each problem will depend upon the nature of the trajectories, on whether they intersect ($d\sigma = 0$) and on whether or not $v = 0$ on them. Furthermore, as was pointed out above, it is necessary to make a special study of the solution on the caustics, where a different asymptotic expansion is required. The methods which have been used in electromagnetic theory seem to be appropriate for this problem, but will not be discussed further here. It should be mentioned that the relationship between the values of P on the two sides of a caustic is analogous to the " connection" problem at a turning point in the WKB method.

Finally it is to be noted from (15) to (17) that $\hbar$ and n enter the solution only in the combination $n\hbar$. In some problems the solution for fixed n does not have the asymptotic behavior assumed in the derivation. However when the double limit in which n becomes infinite while $\hbar$ becomes zero and $n\hbar$ is constant is considered, the assumed asymptotic behavior may result. In this case the asymptotic solution applies only for high quantum numbers n.

APPENDIX

The "Classical ψ Function" for Rutherford Scattering

Consider the quantum mechanical scattering of a charged particle of mass m, charge e and initial momentum p by a fixed particle of charge Ze. Since the energy E of the system is constant, it is equal to the initial kinetic energy of the particle $\frac{p^2}{2m}$. Thus ψ satisfies the time-independent Schroedinger equation

$$\text{(A-1)} \qquad -\frac{\hbar^2}{2m}\nabla^2\psi + \left(\frac{Ze^2}{r} - \frac{p^2}{2m}\right)\psi = 0.$$

The origin of coordinates is taken at the fixed particle. If the incident particle comes from the left, it is represented by the plane wave $A_o \exp(ip\hbar^{-1}x)$. Thus ψ should consist only of outgoing waves in addition to the plane wave, which will itself be modified by the potential.

The "classical ψ function" ψ_o can be constructed by means of (11) and (14), if we first determine the classical trajectories of a particle with momentum p in the potential of the fixed charge Ze at the origin. Since these trajectories are plane curves - in fact hyperbolas - they can be described in terms of the polar coordinates r and Θ by the equation

$$\text{(A-2)} \qquad r^{-1} = \frac{1}{ab^2}\left[1 + \epsilon\cos(\Theta - \omega)\right].$$

Here b is the "impact parameter" and a, ϵ, ω are constants defined by

$$\text{(A-3)} \qquad a = \frac{2E}{Ze^2}, \quad \epsilon = \sqrt{1 + a^2b^2}, \quad \tan\omega = ab.$$

Equation (A-2) describes a hyperbola of eccentricity ϵ with one asymptote given by $y = r \sin \Theta = b$, which represents the incoming path of the particle. The other asymptote, representing the outgoing path, is $\Theta = \phi$, where

(A-4) $$\tan \phi/2 = -\frac{1}{ab} \, .$$

To compute S we note that from the Hamilton-Jacobi equation,

(A-5) $$|\nabla S| = \left(p^2 - \frac{2mZe^2}{r}\right)^{1/2} .$$

Since the direction of ∇S is along the trajectories, we have on each trajectory

(A-6) $$S(r,b) = S_o(b) \pm \int_{r_o}^{r} \left(p^2 - \frac{2mZe^2}{r}\right)^{1/2} d\ell \, .$$

Here $d\ell = \left(1 + r^2 \left[\frac{dr}{d\Theta}\right]^{-2}\right)^{1/2} dr$ is the element of arclength along a trajectory, r_o is the minimum value of r on the trajectory, and $S_o(b)$ is the value of $S(r,b)$ at r_o. The minus sign is to be chosen on the "incident" side of r_o and the plus sign on the "outgoing" side. The value $S_o(b)$ is determined by the condition that $S(r,b)$ must approach px as r becomes infinite on the incident side of the trajectory, in accordance with the "boundary" condition. If we make use of (A-2), (A-6) becomes

(A-7) $$S(r,b) = S_o(b) \pm \int_{r_o}^{r} \left(p^2 - \frac{2mZe^2}{r}\right)^{1/2} \left(1 + \frac{a^2b^4}{\epsilon^2 r^2 \left[1-(ab^2\epsilon^{-1}r^{-1}-\epsilon^{-1})^2\right]}\right)^{1/2} dr.$$

To determine the behavior of $S(r,b)$ as r becomes infinite, we may calculate the asymptotic value of the integral for large r. This calculation leads to the result

$$\text{(A-8)} \qquad S(r,b) = S_o(b) \pm \left[pr - \frac{mZe^2}{p} \log r + C(b) + \cdots \right].$$

In (A-8) C(b) is a constant. Thus we see that $S_o(b)$ must be set equal to C(b) in order to satisfy the "boundary condition". The logarithmic term in (A-8) is the same as that obtained in the exact solution of the Schroedinger equation.

In order to compute A(r,b) we make use of (14), which yields, in view of the rotational symmetry of the present problem about the x-axis,

$$\text{(A-9)} \qquad A^2(r,b) = \frac{A_o^2 v_o b\,db}{v \cdot r \sin\theta \cdot r\,d\theta \; \left(1 + r^2 \left|\frac{dr}{d\theta}\right|^{-2}\right)^{1/2}}$$

$$= A_o^2 p \left(p^2 \; \frac{2mZe^2}{r}\right)^{1/2} \; \frac{b}{r^2 \sin\theta} \left(\omega_b + \epsilon^{-1} \epsilon_b \cot(\theta - \omega) - \frac{2\epsilon b}{r\epsilon \sin(\theta - \omega)}\right)^{-1}$$

$$\cdot \left(1 + \frac{a^2 b^4}{\epsilon^2 r^2 \sin^2(\theta - \omega)}\right)^{-1/2}.$$

The above expression yields an infinite value for A on the caustic curve, defined by $\theta_b = 0$. Thus on and near this curve the present asymptotic expansion fails.

To obtain the asymptotic behavior of A(r,b) for large r on the outgoing part of the trajectory, we note that θ approaches ϕ as r becomes infinite. Then θ_b approaches ϕ_b and one obtains from (A-9)

$$\text{(A-10)} \qquad A^2(r,b) = \frac{A_o^2}{r^2 4\epsilon^2 \sin^4 \phi/2} + \cdots.$$

Equation (A-10) yields an asymptotic value of the amplitude which coincides with that obtained by solving the Schroedinger equation exactly, as is well known.

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